Prandtl number effects in MRT lattice Boltzmann models for shocked and unshocked compressible fluids

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Abstract This paper constructs a new multiple relaxation time lattice Boltzmann model which is not only for the shocked compressible fluids, but also for the unshocked compressible fluids. To make the model work for unshocked compressible fluids, a key step is to modify the collision operators of energy flux so that the viscous coefficient in momentum equation is consistent with that in energy equation even in the unshocked system. The unnecessity of the modification for systems under strong shock is analyzed. The model is validated by some well-known benchmark tests, including thermal Couette flow, Riemann problem. The first system is unshocked and the latter is shocked. In both systems, the Prandtl number effects are checked. Satisfying agreements are obtained between new model results and analytical ones. [doi:10.1063/2.1105204]

Keywords lattice Boltzmann method, compressible flows, multiple-relaxation-time, Prandtl number

In recent years, the lattice Boltzmann (LB) method has attracted much attention as a powerful tool in direct numerical simulation of fluid flows.[1–7] However, there are also some limitations which restrict the applications of traditional LB method, such as the numerical stability problem, the fixed Prandtl number, and so on. To overcome these problems, an effective method is the multiple relaxation time (MRT) LB method,[8–11] which employs multiple relaxation parameters in the collision step, instead of the commonly used Single Relaxation Time (SRT) collision. The flexibility gained from the MRT collision can be used to improve the stability property and overcomes the fixed Prandtl number problem.

To the authors' knowledge, most of the existing MRT LB models work only for isothermal system,[12–15] to cite but a few. To simulate system with temperature field, Luo et al.[16] suggested a hybrid thermal MRT LB model, in which the mass and momentum equations are solved by the MRT model, whereas the diffusion-advection equation for the temperature is solved by Finite Difference (FD) technique or other means. Guo et al.[17] proposed a coupling MRT LB model for thermal flows with viscous heat dissipation and compression work. Mezrhab et al.[18] proposed a double MRT LB method, where MRT-D2Q9 model and the MRT-D2Q5 model are used to solve the flow and the temperature fields, respectively.

Besides the models mentioned above, we have proposed two MRT FD LB models for compressible fluids under shock in previous work.[19,20] Numerical experiments showed that compressible flows with strong shocks can be well simulated by these models. In this paper, we further propose a new MRT LB model, which is not only for the shocked compressible fluids, but also for the unshocked compressible fluids.

The evolution of the distribution function f_i is governed by the following equation

$$\frac{\partial f_i}{\partial t} + v_{i\alpha}\frac{\partial f_i}{\partial x_\alpha} = -M_{il}^{-1}\hat{S}_{lk}(\hat{f}_k - \hat{f}_k^{\mathrm{eq}}), \tag{1}$$

where the matrix $\hat{\boldsymbol{S}} = \boldsymbol{MSM}^{-1} = \mathrm{diag}(s_1, s_2, \cdots, s_N)$ is the diagonal relaxation matrix, f_i and $\hat{f}_i$ are the particle distribution function in the velocity space and the kinetic moment space respectively, $\hat{f}_i = m_{ij}f_j$, m_{ij} is an element of the transformation matrix $\boldsymbol{M}$. $\boldsymbol{M} = (m_1, m_2, \cdots, m_N)^{\mathrm{T}}$, $m_i = (m_{i1}, m_{i2}, \cdots, m_{iN})$. We construct a two-dimensional MRT LB model based on a 16 -discrete-velocity model (see Fig. 1):

$$(v_{i1}, v_{i2}) = \begin{cases} \mathrm{cyc}: (\pm 1, 0), & \text{for } 1 \le i \le 4, \\ (\pm 1, \pm 1), & \text{for } 5 \le i \le 8, \\ \mathrm{cyc}: (\pm 2, 0), & \text{for } 9 \le i \le 12, \\ (\pm 2, \pm 2), & \text{for } 13 \le i \le 16, \end{cases}$$

where cyc indicates the cyclic permutation.

The transformation matrix $\boldsymbol{M}$ is constructed according to the irreducible representation bases of SO(2) group.[20] Using the Chapman-Enskog expansion[13,14,21] on the two sides of LB equation, we can derive the Navier-Stokes (NS) equations for compressible fluids[20]

$$\frac{\partial \rho}{\partial t} + \frac{\partial j_\alpha}{\partial x_\alpha} = 0, \tag{2a}$$

$$\frac{\partial j_\alpha}{\partial t} + \frac{\partial (j_\alpha j_\beta/\rho)}{\partial x_\beta} = -\frac{\partial P}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta}\left[\mu\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta}\right)\right]. \tag{2b}$$

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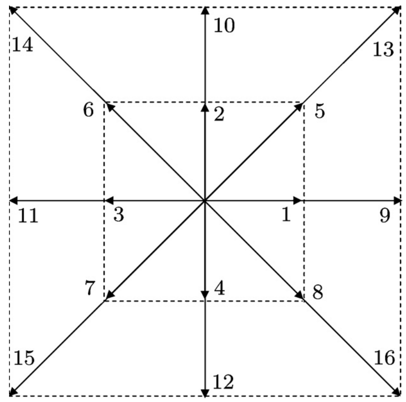

Fig. 1. Schematic diagram of $\boldsymbol{v}_i$ for the discrete velocity model.

$$\frac{\partial e}{\partial t}+\frac{\partial}{\partial x_\alpha}[(e+P)j_\alpha/\rho]=\frac{\partial}{\partial x_\alpha}\left\{\lambda\left[R\frac{\partial T}{\partial x_\alpha}+\frac{1}{2}u_\beta\left(\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}-\frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta}\right)\right]\right\}. \tag{2c}$$

where $\mu=\rho RT/s_5=\rho RT/s_6$, $\lambda=2\rho RT/s_7=2\rho RT/s_8$. The transformation matrix and equilibrium functions of the non-conserved moments are shown in Appendix.

It should be pointed out that, the viscous coefficient in Eq. (2c) is not consistent with that in Eq. (2b). Motivated by the idea of Guo et al.[17], the collision operators of the moments related to the energy flux are modified as

$$\hat{S}_{77}(\hat{f}_7-\hat{f}_7^{\mathrm{eq}})\Rightarrow\hat{S}_{77}(\hat{f}_7-\hat{f}_7^{\mathrm{eq}})+(s_7/s_5-1)\rho Tu_x\cdot\left(\frac{\partial u_x}{\partial x}-\frac{\partial u_y}{\partial y}\right)+(s_7/s_6-1)\rho Tu_y\cdot\left(\frac{\partial u_y}{\partial x}+\frac{\partial u_x}{\partial y}\right),$$

$$\hat{S}_{88}(\hat{f}_8-\hat{f}_8^{\mathrm{eq}})\Rightarrow\hat{S}_{88}(\hat{f}_8-\hat{f}_8^{\mathrm{eq}})+(s_8/s_6-1)\rho Tu_x\cdot\left(\frac{\partial u_y}{\partial x}+\frac{\partial u_x}{\partial y}\right)-(s_8/s_5-1)\rho Tu_y\cdot\left(\frac{\partial u_x}{\partial x}-\frac{\partial u_y}{\partial y}\right).$$

With this modification, we are able to get the following energy equation

$$\frac{\partial e}{\partial t}+\frac{\partial}{\partial x_\alpha}[(e+P)j_\alpha/\rho]=\frac{\partial}{\partial x_\alpha}\left[\lambda R\frac{\partial T}{\partial x_\alpha}+\mu u_\beta\left(\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}-\frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta}\right)\right]. \tag{3}$$

This modification method is also suitable for our previous MRT models.[19,20] The definitions of $\hat{f}_{12}^{\mathrm{eq}}$, $\hat{f}_{15}^{\mathrm{eq}}$, $\hat{f}_{16}^{\mathrm{eq}}$ have no effect on macroscopic equations, so the choices of the three moments are flexible. We set $\hat{f}_{12}^{\mathrm{eq}}=\hat{f}_{15}^{\mathrm{eq}}=\hat{f}_{16}^{\mathrm{eq}}=0$.

Here we conduct a series of numerical simulations of Couette flow, to compare the ability of the unmodified model and the modified model for the unshocked compressible fluids. In the simulation, the left wall is fixed and the right wall moves at speed $U=0.1$. The initial state of the fluid is $\rho=1$, $T=1$, $U=0$. The simulation results are compared with the analytical solution

$$T=T_1+(T_2-T_1)\frac{x}{H}+\frac{\mu}{2\lambda}U^2\frac{x}{H}\left(1-\frac{x}{H}\right),$$

where T_1 and T_2 are the left and right wall's temperatures ($T_1=1$, $T_2=1.005$), H is the width of the channel. Periodic boundary conditions are applied to the bottom and top boundaries, the left and right walls adopt the nonequilibrium extrapolation method. Figures 2 and 3 show the temperature profiles of Couette flow simulated with the unmodified model and its modified version. In Fig. 2, we fix viscosity coefficient $s_5=s_6=10^3$, and change the thermal conductivity $s_7=s_8$ from 10 to 2×10^3. On the contrary, we fix thermal conductivity $s_7=s_8=10^3$, and change the viscosity $s_5=s_6$ from 10^2 to 10^3, Fig. 3(a) corresponds to the unmodified model, Fig. 3(b) corresponds to the modified model. It is clearly shown that the simulation results of modified model are in agreement with the analytical solutions, and the Prandtl number effects on unshocked compressible fluids are successfully captured by the modified model, but not by the unmodified model.

Here we construct a high Mach number shock tube problem with the initial condition

$$\begin{aligned}&(\rho,u_1,u_2,T)|_L=(5.0,45.0,0.0,10.0),\ x\le0,\\&(\rho,u_1,u_2,T)|_R=(6.0,-20.0,0.0,5.0),x>0.\end{aligned} \tag{4}$$

The Mach number of the left side is 10.1 ($Ma=u/\sqrt{2T}=45/\sqrt{20}$), and the right is 6.3 ($Ma=u/\sqrt{2T}=20/\sqrt{10}$). Figure 4 shows the comparison of LB results and exact solutions at $t=0.018$, where the parameters are $\mathrm{d}x=\mathrm{d}y=0.003$, $\mathrm{d}t=10^{-5}$, $s_5=s_6=1.5\times10^4$, other values of s are 10^5. Squares correspond to simulation results with the unmodified model, the circle symbols correspond to the modified MRT simulation results, and solid lines represent the exact solutions. It can be seen that the simulations of the two MRT models do not show large differences. For shocked compressible flows, there exist a fast procedure and a slow one. The shock dynamic procedure is fast, while that of heat conduction is slow. In such a case, from the viewpoint of macroscopic description, the terms related to viscosity and heat conductivity may be neglected. So, terms related to viscosity and heat conductivity in Eqs. (2b) and (2c) are all small terms and make negligible effects. That is the reason why the unmodified model works also well in such cases.

As a conclusion, we propose an MRT LB model which works not only for the shocked compressible fluids but also for the unshocked compressible fluids. In

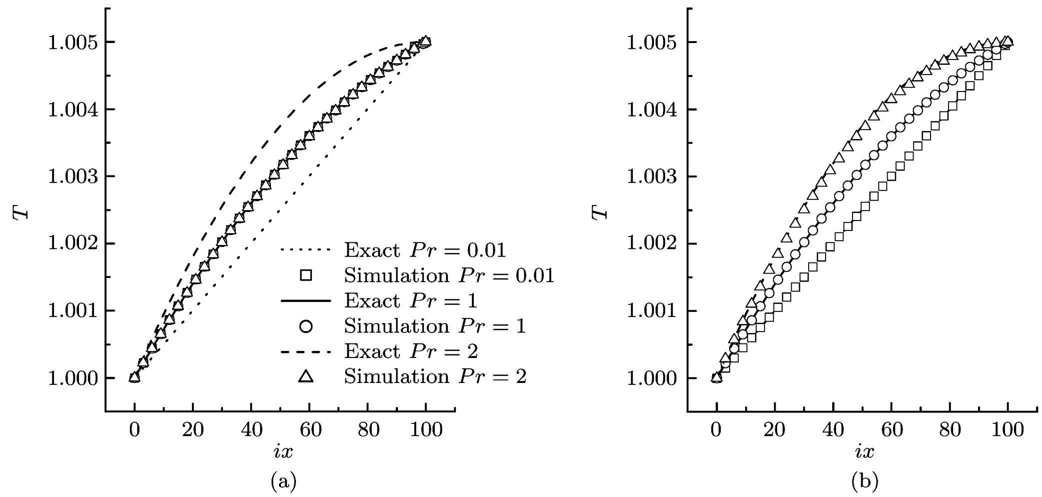

Fig. 2. Effects of heat conductivity on temperature profiles of Couette flow: (a) corresponds to the unmodified model; (b) corresponds to the modified model. The $Pr = 0.01$, $Pr = 1$ and $Pr = 2$ correspond to $s_7 = s_8 = 10$, $s_7 = s_8 = 10^3$, and $s_7 = s_8 = 2 \times 10^3$, respectively (other collision parameters are 10^3).

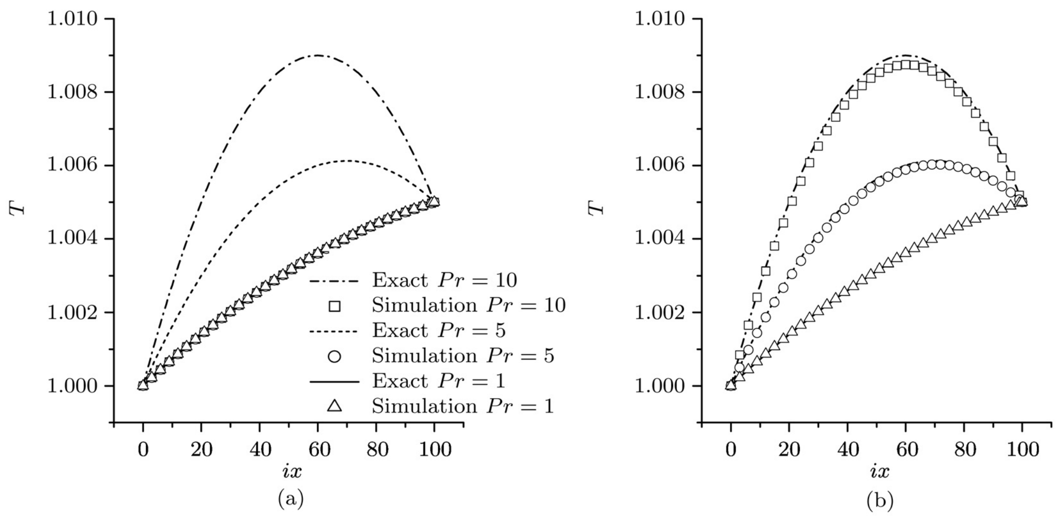

Fig. 3. Effects of viscosity on temperature profiles of Couette flow: (a) corresponds to the unmodified model; (b) corresponds to the modified model. The $Pr = 10$, $Pr = 5$ and $Pr = 1$ correspond to $s_5 = s_6 = 10^2$, $s_5 = s_6 = 2 \times 10^2$, and $s_5 = s_6 = 10^3$, respectively (other collision parameters are 10^3).

the new model, a key step is the modification of the collision operators of energy flux so that viscous coefficient in momentum equation and that in energy equation are consistent no matter if the system is shocked or not. The unnecessity of the modification for systems under strong shock is analyzed. The new model is validated by some well-known benchmark tests, including (1) thermal Couette flow, (2) Riemann problem. The first system is unshocked and the latter is shocked. In both systems, the Prandtl number effects are checked. Satisfying agreements are obtained between the new model results and analytical ones. Our previous models[19,20] can be revised in the same way to simulate unshocked compressible flows.

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APPENDIX: CONSTRUCTION OF THE TRANSFORMATION MATRIX AND $\hat{f}_i^{\mathrm{eq}}$

The transformation matrix $\boldsymbol{M}$ can be expressed as follows: $\boldsymbol{M} = (m_1, m_2, \cdots, m_{16})^{\mathrm{T}}$, where $m_{1i} = 1$, $m_{2i} = v_{ix}$, $m_{3i} = v_{iy}$, $m_{4i} = (v_{ix}^2 + v_{iy}^2)/2$, $m_{5i} = v_{ix}^2 - v_{iy}^2$, $m_{6i} = v_{ix}v_{iy}$, $m_{7i} = v_{ix}(v_{ix}^2 + v_{iy}^2)$, $m_{8i} =$

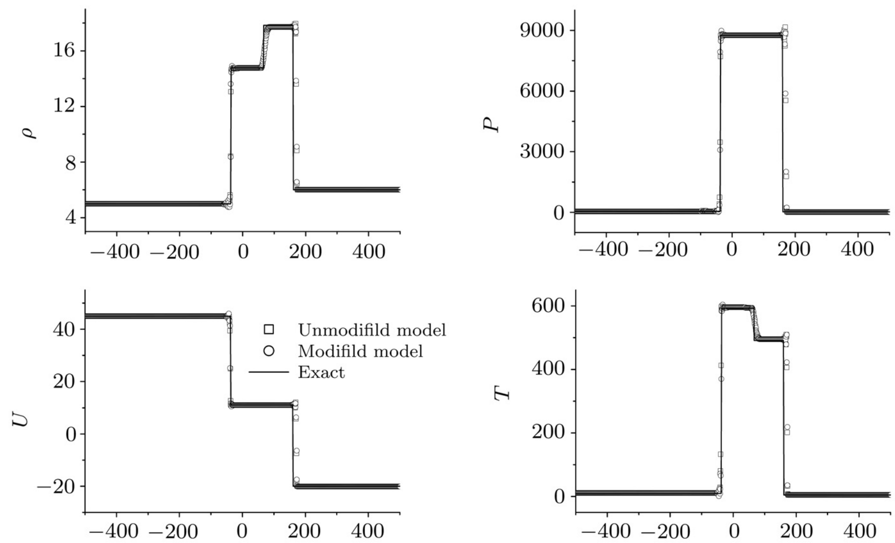

Fig. 4. The LB results and exact solutions for shock tube problem at time $t = 0.018$. ρ: density, P: pressure, U: the $x-$ component of velocity, T: temperature.

$v_{iy}(v_{ix}^2 + v_{iy}^2)$, $m_{9i} = v_{ix}(v_{ix}^2 - 3v_{iy}^2)$, $m_{10i} = v_{iy}(3v_{ix}^2 - v_{iy}^2)$, $m_{11i} = (v_{ix}^2 + v_{iy}^2)^2/4$, $m_{12i} = v_{ix}^4 - 6v_{ix}^2 v_{iy}^2 + v_{iy}^4$, $m_{13i} = (v_{ix}^2 + v_{iy}^2)(v_{ix}^2 - v_{iy}^2)$, $m_{14i} = (v_{ix}^2 + v_{iy}^2)v_{ix}v_{iy}$, $m_{15i} = v_{ix}(v_{ix}^2 + v_{iy}^2)(v_{ix}^2 - 3v_{iy}^2)$, $m_{16i} = v_{iy}(v_{ix}^2 + v_{iy}^2)(3v_{ix}^2 - v_{iy}^2)$, where $i = 1, 2, \cdots, 16$.

The equilibria of the nonconserved moments can be chosen as $\hat{f}_5^{\rm eq} = (j_x^2 - j_y^2)/\rho$, $\hat{f}_6^{\rm eq} = j_x j_y/\rho$, $\hat{f}_7^{\rm eq} = (e + \rho RT)j_x/\rho$, $\hat{f}_8^{\rm eq} = (e + \rho RT)j_y/\rho$, $\hat{f}_9^{\rm eq} = (j_x^2 - 3j_y^2)j_x/\rho^2$, $\hat{f}_{10}^{\rm eq} = (3j_x^2 - j_y^2)j_y/\rho^2$, $\hat{f}_{11}^{\rm eq} = 2e^2/\rho - (j_x^2 + j_y^2)^2/4\rho^3$, $\hat{f}_{13}^{\rm eq} = (6\rho e - 2j_x^2 - 2j_y^2)(j_x^2 - j_y^2)/\rho^3$, $\hat{f}_{14}^{\rm eq} = (6\rho e - 2j_x^2 - 2j_y^2)j_x j_y/\rho^3$.

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